# Stability of Energy Transfer in the Weak Coupling Method

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**Summary.** In this paper we are concerned with a weak coupling technique for the concurrent simulation of multiscale phenomena. In particular we focus on the construction of an initial embedding of discrete atomic data fields in an appropriate subspace $\mathcal{H}_N(\Omega) \subset L^2(\Omega)$ which provides the foundation for the proposed coupling technique in a function space setting. Thus, we must consider the regularity of the coupling information and the stability of the resulting basis.

**Key words:** multiscale, weak coupling, molecular dynamics, continuum mechanics

## 1 Introduction

In many physical phenomena, the macroscopic behavior of solids in structural dynamics is governed by effects on a microscopic scale. As a consequence an accurate representation of large scale behavior requires to capture the effects of all scales from micro to macro. On the macroscopic level a description by continuum mechanics can be used. Since those macroscopic models are usually based on a partial differential equation (PDE), they are –at least formally– incompatible with the discrete displacements on an atomistic level. On the fine scale, models involving detailed information about crystalline and defect structure, such as molecular dynamics yield satisfactory accuracy. Here the interactions are defined by inter atomic potentials. These microscopic mechanics are non-linear and strongly non-local. In contrast to continuum mechanics the description is based on a system of ODEs associated with discrete points in the Euclidean space. However, a complete fine scale description of the problem on the complete macroscopic domain is often computationally infeasible. Thus multiscale models must be employed, where different models are used simultaneously within a single simulation process. Due to the coupling of different effects on the different scales, the development of these methods is a demanding task.

The different multiscale methods vary not only in scope and the underlying assumptions, but also in their approach to broader questions such as a hierarchically and concurrent multiscale approach. In the first class, the computations are performed on each scale separately. Often, the scale coupling is done by transferring problem parameters, i.e., the results obtained on one scale determine the parameters for the computational model on another scale [1, 5]. Thus for instance a continuum model can be derived from the atomic information [2]. Another approach is pursued in the concurrent coupling techniques. Here, computations on different scales are carried out simultaneously [4, 16, 17]. For a recent overview on multiscale techniques we refer to [14].

As afore mentioned, depending on the scale of interest, the relevant dynamics may require the use of quite different models on the respective scales.

Let us consider a displacement field $\nu \in \mathcal{H}_N(\Omega)$, where $\mathcal{H}_N(\Omega)$ is a linear subspace of $L^2(\Omega)$ and $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, is a domain. Here, the displacement field $\nu$ is determined by coarse as well as fine influences. In our multiscale context, we now aim at a decomposition of $\nu$, which separates the high frequency components $\nu'$ of the total solution $\nu$ described by the atomic interactions from the smooth part $\bar{\nu}$ of the displacements. We therefore follow the approach of [9], where in the space $L^2(\Omega)$ the total displacement field $\nu \in \mathcal{H}_N(\Omega)$ is decomposed as

$$\nu = \bar{\nu} + \nu' \,. \tag{1.1}$$

Here, $\bar{\nu}$ is the coarse part of the total displacement and $\nu'$ refers to the fine scale displacements. Let us note that we have chosen a function space oriented setting, since this allows for more flexible decomposition approaches.

As a matter of fact, in case of molecular dynamics, the material behavior on the micro or fine scale is modeled by means of an system of isolated atoms or molecules. More precisely, on the micro scale the atoms $x_\alpha$ and their "discrete displacements" $\tilde{\nu}_\alpha$ form the scattered data set

$$\chi_N(\Omega) := \{(x_\alpha, \tilde{\nu}_\alpha) \,|\, \alpha = 1, ..., N,\, x_\alpha \in \Omega \,, \tilde{\nu}_\alpha \in \mathbb{R}^d\} \,. \tag{1.2}$$

We note that since $\tilde{\nu} \in \mathbb{R}^{dN}$, the atomic displacements on the fine scale cannot be interpreted as an element of $\mathcal{H}_N(\Omega)$. As a consequence, a direct sum decomposition of the underlying function space as in [9] is not possible. This is due to the fact, that the coarse scale values $\bar{\nu}$ are given as a displacement field in $L^2(\Omega)$, whereas the displacement field of the fine scale is given in terms of (1.2).

In the Bridging Scale Method [16] the decomposition given by (1.1) is the starting point for the multiscale simulation. Here, the decomposition is performed in a completely discrete setting. To do so an interpolation operator evaluating an interpolation function at the equilibrium position of the underlying atoms is used. The coarse scale is then the image of a projection from the fine scale displacement onto a displacement field.

In this paper, we pursue a different approach by performing the scale decomposition of the total displacement also for the atomic displacements in $L^2(\Omega)$. At a first glance this function space oriented decomposition seems impossible, since the displacement on the fine scale $\tilde{\nu}$ is given by (1.2). We therefore interpret the discrete displacements $\tilde{\nu} \in \mathbb{R}^{dN}$ as elements of the function space $\mathcal{H}_N(\Omega)$. This is done by means of the linear operator

$$\iota \colon \chi_N(\Omega) \to \mathcal{H}_N(\Omega) \subset L^2(\Omega)\,, \qquad \iota(\tilde{\nu}) = \nu. \tag{1.3}$$

This embedding can be chosen in a problem-dependent fashion and the properties of the resulting multiscale decomposition depend strongly on the choice of a basis $\{\phi_\alpha\}$ for $\mathcal{H}_N(\Omega)$.

For the discretization of the coarse scale we choose linear finite elements. Let $\mathcal{S}^h$ be a finite element space over $\Omega$ related to a mesh $\mathcal{T}_h$. In order to identify the coarse scale displacement $\bar{\nu}$, we employ an $L^2$-projection $\pi : \mathcal{H}_N(\Omega) \to \mathcal{S}^h$. This projection is designed to extract from the total displacement $\nu$ the coarse part, which is assumed to be in the finite element space $\mathcal{S}^h$. More precisely, for any total displacement $w \in \mathcal{H}_N(\Omega)$, the corresponding coarse scale displacement is given by $\pi(w) \in \mathcal{S}^h$ which satisfies

$$(\pi(w), \mu)_{L^2(\Omega)} = (w, \mu)_{L^2(\Omega)} \qquad \forall \mu \in M^h, \tag{1.4}$$

where $M^h$ denotes a suitable multiplier space. In order to compute the algebraic representation of $\pi$ in (1.4), we need to assemble two (generalized) mass matrices. For the first matrix, we need to evaluate integrals of the form $\int_\Omega \mu_p \lambda_q \, dx$, where $\mu_p$ are the basis functions spanning the multiplier space $M^h$, and $\lambda_q$ are the basis functions of $\mathcal{S}^h$. Here, $p, q$ are assumed to be in some index set $\mathcal{N}^h$ with $|\mathcal{N}_h| = \dim(\mathcal{S}^h)$. The computation of the resulting mass matrix can be done in a similar fashion as the assembly of the standard mass matrix. For the second matrix, we need to evaluate integrals of the form

$$\int_\Omega \mu_p \phi_\alpha \, dx \tag{1.5}$$

where the $\phi_\alpha$ are the basis functions for the space $\mathcal{H}_N(\Omega)$, i.e. $\mathcal{H}_N(\Omega) = \operatorname{span}\langle\phi_\alpha\rangle$. In order to compute these integrals the intersection between the support of $\mu_p$ and the support of $\phi_\alpha$ has to be computed. For details concerning an efficient way for computing these intersections, we refer to [7].

Summing up the weak coupling concept involves several steps: In the first step, an approximation of the fine scale displacement embeds the discrete values into a function space. In the second step we perform an $L^2$-like projection separating the coarse from the fine scale. In case the molecular dynamic simulation is restricted to a subset of $\Omega$, in a third and final step, the resulting low-frequency contributions have to be extended to the whole computational domain $\Omega$. For further details we refer to [6].

In the forthcoming we examine the first step of our transfer scheme, namely the operator $\iota$. A possible choice for $\iota$ could be $\iota(\tilde{\nu}) = \sum_\alpha \tilde{\nu}_\alpha \phi_\alpha$. For this choice, we need to specify "suitable" basis functions $\phi_\alpha$. In the context of multiscale methods the term suitable refers to the kind of information which we are interested in. More precisely we can expect that for the transfer of gradient based information from the fine to the coarse scale a basis which can only reproduce constants exactly is insufficient. Thus, for the construction of these basis functions, we will employ techniques from scattered data approximation which allow for a flexible choice of the basis functions $\phi_\alpha$.

One class of shape function used for scattered data interpolation are the radial basis functions [10]. Another approach to construct shape functions $\phi_\alpha$ from the collection of particles $\chi_N(\Omega)$ is based in the moving least squares technique (MLS) that we shortly summarize in the next section, see e.g. [8] for details.

## 2 Moving Least Squares Method

Here, we construct the operator $\iota$ from (1.3) on the basis of the moving least squares approach which originated in scattered data approximation. We suppose, that the scattered data set $\chi_N(\Omega)$ in (1.2) is given. Our aim is to find a function $u : \bar{\Omega} \to \mathbb{R}$, such that

$$u(x_\alpha) \approx \tilde{\nu}_\alpha \text{ for all } \alpha = 1, ..., N. \tag{2.6}$$

In order to construct a moving least squares (MLS) fit, we consider the approximation space being the space $\mathbb{P}_m$ of polynomials with the basis $\{P_i\}_{i=1}^N$ of degree $m$ in $d$ variables [1] and a set of non-negative weight functions

$$W_\alpha : \mathbb{R}^d \to \mathbb{R}_0^+ \text{ with } \operatorname{supp}(W_\alpha) =: \omega_\alpha,$$

and the dilatation parameter $h_\alpha$ of $W_\alpha(x) = W\left(\frac{x - x_\alpha}{h_\alpha}\right)$. Now, we minimize for each $x$ the quadratic functional

$$J(\tau)(x) = \sum_{\alpha=1}^{N} W_\alpha(x)(\nu_\alpha - \tau(x_\alpha))^2 \tag{2.7}$$

over all $\tau \in \mathbb{P}_m$.

In order to minimize (2.7), we set the derivative of (2.7) equal to zero and obtain the system of equations

$$\sum_{\alpha=1}^{N} W_\alpha(x)\tilde{\nu}_\alpha P_j(x_\alpha) = \sum_{\alpha=1}^{N} W_\alpha(x) \sum_{i=1}^{n} P_i(x_\alpha) P_j(x_\alpha) c(x) \qquad j = 1, ..., n. \tag{2.8}$$

[1] The approximation space can be generalized to an abstract approximation space $V(\Omega)$. Note however, that we then obtain reproduction of $V(\Omega)$ by $\phi_\alpha$ of (2.11).

With the definitions

$$\begin{aligned} P(x) &:= [P_1(x)\ P_2(x)\ \cdots\ P_N(x)]^T \\ W(x) &:= [W_1(x)\ W_2(x)\ \cdots\ W_N(x)]^T \\ B &:= (B_{ij})_{i,j=1,\ldots,N},\ B_{ij} = W_i(x)P_j(x) \\ f &:= [\tilde{\nu}_1\ \tilde{\nu}_2\ \cdots\ \tilde{\nu}_N]^T \\ A(x) &:= (A_{ij})_{i,j=1,\ldots,n},\ A_{ij} = \sum_{\alpha=1}^{N} P_i(x_\alpha)W_\alpha(x)P_j(x_\alpha) \\ c(x) &:= [c_1(x)\ c_2(x)\ \ldots\ c_n(x)]^T, \end{aligned}$$

equation (2.8) can be written as

$$A(x)c(x) = B(x)f. \tag{2.9}$$

The above matrix $A(x)$ is also known as Gram's matrix. The minimizer $u(x)$ f (2.7) is given by the linear combination

$$u(x) = \sum_{\alpha=1}^{N} \tilde{\nu}_\alpha \phi_\alpha(x) \tag{2.10}$$

where the shape functions $\phi_\alpha$ satisfy

$$\phi_\alpha(x) = P^T(x_\alpha)[A(x)]^{-1}W_\alpha(x)P(x_\alpha). \tag{2.11}$$

*Properties of the Gram-Matrix*

Note that (2.11) involves the inverse of the Gram matrix $A(x)$ for each point of evaluation. Thus, we must be concerned with the regularity of $A(x)$ for all $x \in \Omega$. Here, we attain the positive definiteness of $A(x)$ for all $x \in \Omega$ from the $\mathbb{P}_m$-unisolvence of the sets $\chi_N(\Omega) \cap \omega_\alpha$ for all $\alpha$.

*Weight Functions and Scaling*

The size of the support of the weight functions $W_\alpha$, i.e. of the shape functions $\phi_\alpha$ can be determined by

$$\omega_\alpha = \{y \in \mathbb{R}^d \mid \|x_\alpha - y\| < h_\alpha\}$$

where the dilatation parameter $h_\alpha$ can in principle be chosen individually for each data site $x_\alpha$. However, this choice is closely related to the accuracy and stability of the approximation and thus crucial for the stability of the projection operator $\pi$. Recall that the $\mathbb{P}_m$-unisolvence of $\chi_N(\Omega) \cap \omega_\alpha$ for all $\alpha$ must be ensured. Note also that the smoothness of the approximation depends on the smoothness of the weight function, i.e. if $W_\alpha \in C^r(\Omega)$ then $\phi_\alpha \in C^r(\Omega)$.

*Reproduction Properties*

¿From (2.10) with $\nu_\alpha = u(x_\alpha)$ for $u \in \mathbb{P}_m$ and (2.11) it is clear that $\mathbb{P}_m \subset \text{span}\langle\phi_\alpha\rangle$, thus reproduction of polynomials of order $m$ in MLS is guaranteed.

*Partition of Unity and Shepard's Approach*

We denote $\{\phi_\alpha\}$ as a partition of unity of order $q$ if the reproducing property

$$\sum_{\alpha=1}^{N} \phi_\alpha(x) b(x_\alpha) = b(x)$$

and the derivative reproducing conditions

$$\sum_{\alpha=1}^{N} D^s \phi_\alpha(x) b(x_\alpha) = D^s b(x), \quad |s| \leq q$$

hold for all $b \in \mathbb{P}_m$. In the case of $m = 0$, the approximation space is given by $\mathbb{P}_m = \{\mathbf{1}\}$ and the Gram matrix reduces to

$$A(x) = \sum_{\alpha=1}^{N} W_\alpha(x).$$

Thus the shape functions are given by

$$\phi_\beta(x) = \frac{W_\beta(x)}{\sum_{\alpha=1}^{N} W_\alpha(x)} = W(x) \cdot (A(x))^{-1}$$

which is also known as Shepard's method. One can thus easily verify, that

$$0 < \phi_\beta(x) < 1 \;\text{ and }\; \sum_{\beta=1}^{N} \phi_\beta(x) = 1 \;\forall x \in \Omega.$$

The Shepard partition of unity is an efficient method for the approximation of scattered data, since the Gram matrix reduces to a scalar, and thus an explicit form of $\phi_\alpha$ is given. As a drawback, the type of information which we can transfer from a coarse to a fine scale is confined to displacements. For gradient based information a higher order MLS method has to be applied, which requires the implicit representation (2.11).

In general the MLS approximant is non interpolating, i.e. they do not satisfy the Kronecker delta property. However an interpolating approximant can be constructed by using singular weighting functions at all nodes [11].

For the deduction of the MLS shape function we can use different starting points like the minimization of a weighted least-squares functional, or a Taylor-Series expansion, or the direct imposition of the reproducing conditions. There

are also other techniques, which produce a partition of unity like e.g. the Reproducing Kernel Particle Methods (RKPM) [3, 12, 13]. Even though that the RKPM and the MLS have different origins their equivalence can be shown. We want to employ the MLS functions as the basis for our space $\mathcal{H}_N(\Omega)$, i.e. for the range of the embedding. Our construction is essentially $L^2$ based and so Shepard's method should be sufficient to obtain at least first order in $L^2$. If we also need to bound the error in $H^1$ then MLS of first order should be employed.

## 3 Numerical Experiment

To confirm this assertion, we consider the idealized but representative reference scattered data approximation problem (2.6) via the minimization of (2.7) for the data $f_\alpha = u(x_\alpha)$ where $u(x) = x^2$. We compare the results obtained via the MLS approach for the point set $[-3, 3]$ with $h = 1$ using the approximation spaces $\mathbb{P}_m$ with $m = 0, 1$. Here, we anticipate to find an asymptotic convergence behavior of $O(h)$ in the $L^2$-norm for $m = 0$ and $O(h^2)$ for $m = 1$. Furthermore, the approximation error will stagnate with respect to the $H^1$-norm for the Shepard functions with $m = 0$ whereas the MLS shape functions with $m = 1$ will provide an $O(h)$ convergence also in $H^1$. This expected convergence behavior can be clearly observed from Figure 3.2.

Thus, the construction of a weak coupling operator aimed at transferring function values may be based on the Shepard functions (if the error bound of $O(h)$ where $h$ is related to the maximal atomic distance is acceptable), compare Figure 3.1. However, if the transfer of gradient information is required (or the jump in the resolution between coarse function space $\mathcal{S}_h$ and $\mathcal{H}_N(\Omega)$ is too small) the use of higher order moving least squares functions is necessary.

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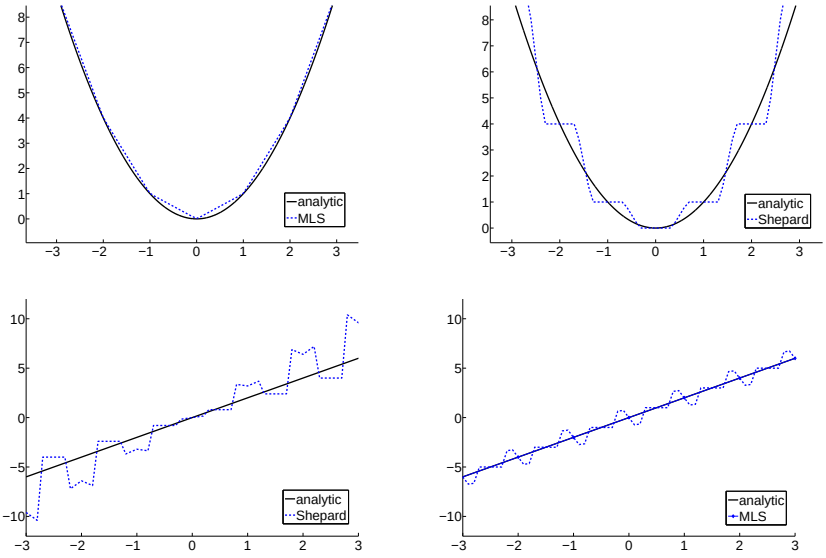


**Figure 3.1.** Approximation (top row) by Shepard's Method (left) and MLS (right) and the respective derivatives (bottom row).

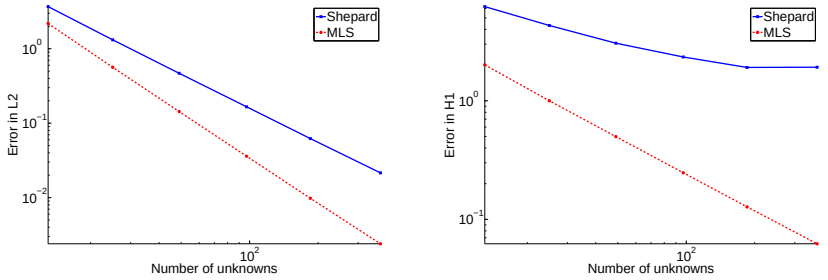


**Figure 3.2.** Error in the $L^2$-norm (left) and $H^1$-norm (right) of Shepard's method (solid) and the MLS (dashed).

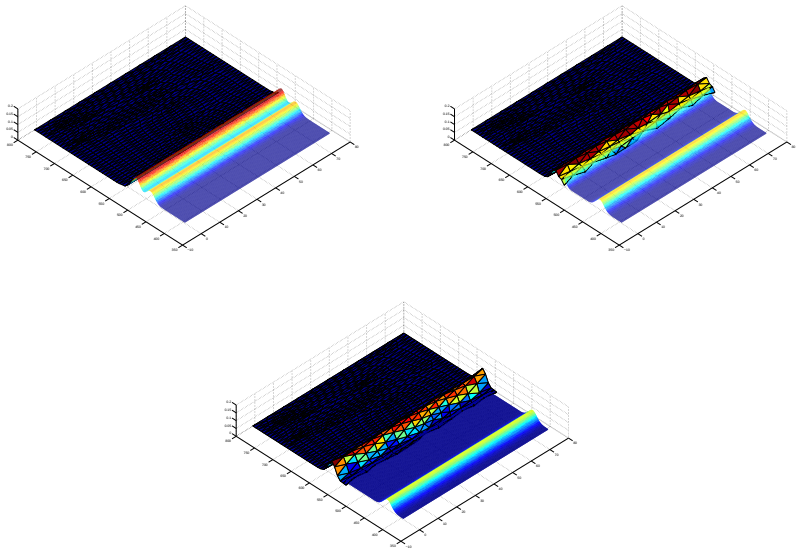

**Figure 3.3.** Weak scale transfer ($2d$) based on (1.4) using Shepard's approach ($m = 0$.


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